

Perhydrotriquinacene

Inchi:

lnChI=1S/C10H16/c1-2-8-5-6-9-4-3-7(1)10(8)9/h7-10H,1-6H2

InchiKey:

MVMFUXACHPDDMY-UHFFFAOYSA-N

Formula:

C10H16

SMILES:

C1CC2CCC3CCC1C23

Mol. weight [g/mol]:

136.23

CAS:

17760-91-7

Physical Properties

Property code	Value	Unit	Source
chs	-6062.80 ± 3.20	kJ/mol	NIST Webbook
gf	195.76	kJ/mol	Joback Method
hf	-102.30 ± 3.60	kJ/mol	NIST Webbook
hfs	-159.00 ± 3.20	kJ/mol	NIST Webbook
hfus	15.03	kJ/mol	Joback Method
hsub	56.70	kJ/mol	NIST Webbook
hvap	37.46	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	2.833		Crippen Method
mcvol	119.180	ml/mol	McGowan Method
pc	3100.18	kPa	Joback Method
tb	448.02	K	Joback Method
tc	661.62	K	Joback Method
tf	248.52	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	364.21	J/mol×K	626.02	Joback Method
cpg	348.41	J/mol×K	590.42	Joback Method
cpg	331.44	J/mol×K	554.82	Joback Method
cpg	313.20	J/mol×K	519.22	Joback Method
cpg	293.60	J/mol×K	483.62	Joback Method
cpg	272.54	J/mol×K	448.02	Joback Method

cpg	378.92	J/mol×K	661.62	Joback Method
dvisc	0.0006121	Pa×s	248.52	Joback Method
dvisc	0.0011052	Pa×s	448.02	Joback Method
dvisc	0.0010419	Pa×s	414.77	Joback Method
dvisc	0.0009721	Pa×s	381.52	Joback Method
dvisc	0.0008951	Pa×s	348.27	Joback Method
dvisc	0.0008100	Pa×s	315.02	Joback Method
dvisc	0.0007158	Pa×s	281.77	Joback Method
hsubt	56.60 ± 1.30	kJ/mol	307.00	NIST Webbook
hsubt	56.60 ± 1.30	kJ/mol	307.00	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17760917&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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